Message

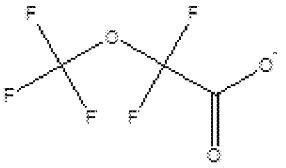
From: Strynar, Mark [/O=EXCHANGELABS/OU=EXCHANGE ADMINISTRATIVE GROUP (FYDIBOHF23SPDLT)/CN=RECIPIENTS/CN=5A9910D5B38E471497BD875FD329A20A-STRYNAR, MARK]
Sent: 4/6/2017 12:22:41 PM
To: Detlef Knappe [knappe@ncsu.edu]
CC: Lindstrom, Andrew [/o=ExchangeLabs/ou=Exchange Administrative Group (FYDIBOHF23SPDLT)/cn=Recipients/cn=04bf7cf26aa44ce29763fbc1c1b2338e-Lindstrom, Andrew]
Subject: RE: PFECA structures

Detlef,

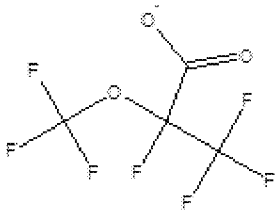
It is really hard to know for sure, and both figures may be correct. Chemspider shows multiple isomers for each formula in this series. I don't think we could separate these short chained isomers to see if multiple forms exist with C8 or C18 columns. Perhaps with HILIC.

However I think the structures in Figure S7 are correct for the first 4 compounds (up to GenX in size). GenX is the only one I can say for sure is correct as drawn below. Thus I think the first 2 in figure S5 are correct, after that (m/z 278.9709 and higher MW) may not be. Not sure why we did not see S5 and S7 had different structures. I expect these are the correct structure below, however I have no way to know.

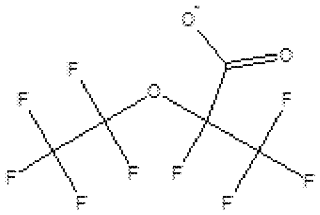
Mark



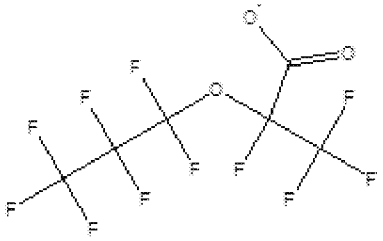
Molecular Formula: $C_5F_9O_2^-$
Monoisotopic Mass: 178.977308 Da



Molecular Formula: $C_6F_9O_2^-$
Monoisotopic Mass: 228.974115 Da



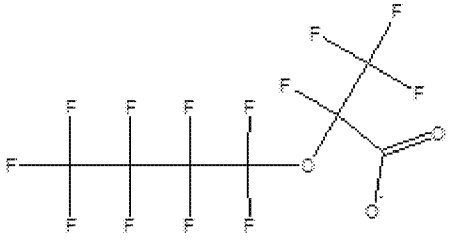
Molecular Formula: $C_6F_9O_3^-$
Monoisotopic Mass: 278.970921 Da



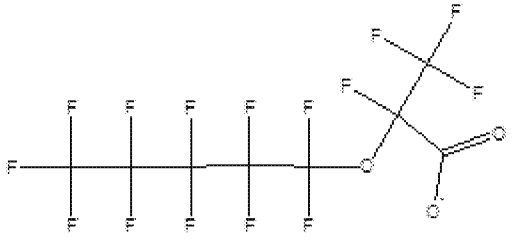
Target Compound CAS # 13252-13-6

GenX

Molecular Formula	= $C_6F_{11}O_3$
Formula Weight	= 329.045838
Composition	= C(21.90%) F(63.51%) O(14.59%)
Monoisotopic Mass	= 328.967728 Da
[M-H]-	= 327.960451 Da



Molecular Formula: $C_7F_{13}O_2^-$
Monoisotopic Mass: 378.964634 Da



Molecular Formula: $C_8F_{15}O_2^-$
Monoisotopic Mass: 428.96134 Da

From: Detlef Knappe [mailto:knappe@ncsu.edu]
Sent: Tuesday, April 04, 2017 8:35 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: RE: PFECA structures

Thank you, Mark. Can you let me know whether there are other structures that might not be right in figure S5?
Detlef

On Apr 4, 2017 12:20 PM, "Strynar, Mark" <Strynar.Mark@epa.gov> wrote:

> Detlef,
>
> In figure S5 I think the structure is not correct from the 2015 SI. These were the suspected structures and we did not QTOFMS data at the time. If these were both correct we could tell them apart with MS/MS as they would likely cleave at the ether oxygen. The top would give a C2F5O (135) transition and the bottom a C3F7O (153) transition for the daughter assuming the O migrates with the fragment. If not we would get a C2F5 (119) and a C3F7 (169) transition respectively.

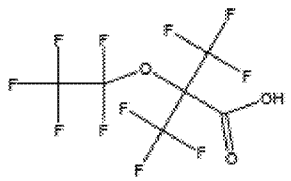
I think they are both GenX and the lower structure is correct.

Mark

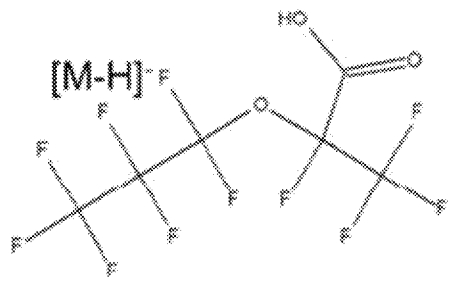
From: Detlef Knappe [mailto:knappe@ncsu.edu]
Sent: Tuesday, April 04, 2017 3:03 PM
To: Strynar, Mark <Strynar.Mark@epa.gov>
Subject: PFECA structures

Mark,

I am struggling with PFECA structures. In your 2015 paper, your homologous series (Figure S5) shows



Can we distinguish the above compound from GenX, which looks like this (same overall formula)



Detlef

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